THE TRACE FORMULAS FOR A HALF-LINE SCHRODINGER OPERATOR WITH LONG-RANGE POTENTIALS

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Abstract.

The present work deals with trace formulas for a half-line Schrödinger operator with long-range potentials. These formulas relate the potential with some scattering data. We generalize some relevant results by Buslaev, Faddeev, Gesztesy, Holden, Simon, and others to the case of square integrable potentials. The relation between the number of the trace formulas and the number of integrable derivatives of the potential is also given.

Contents

Preface.

We study a one-dimensional half-line case with minimal restrictions on the potential. The main interest is in proving so called Buslaev-Faddeev trace formulas. The number of the trace formulas for a given number of integrable derivatives of the potential has been found. Unfortunately, even in such simplified case as a one dimensional problem, only partial results have been obtained. We have discovered only sufficient conditions for trace formulas. This work is an attempt to improve the results of F.Gesztesy, H.Holden and others.

Section 3 contains a proof of the well-known fact of the existence of the solution to a one-dimensional Schrödinger equation with WKB-type asymptotics for the square integrable potential possessing integrable first derivative. The main result of the section is an iterative representation of the solution.

Section 4 contains calculations showing the number of terms of the asymptotic representation of the solution at the origin for large energies that can be written if additionally we assume the existence and integrability of N derivatives of the potential. Here we used the results from the previous section.

Section 5 contains a description of the spectral shift function. This function always appears when one is dealing with the trace formulas. Definitions, basic properties and relevance to the subject are given in this section.

Section 6 contains a proof of the main theorem which states the necessary conditions on the potential to write certain number of Buslaev-Faddeev trace formulas. Also, for the convenience of the reader we provide several first trace formulas with explicitly written coefficient.

1 Introduction.

The study of the Schrödinger operator has a long and rich history [18]. The time-dependent Schrödinger wave equation ($\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + ... + \frac{\partial^2}{\partial x_n^2}$)

$$\left[-\frac{\hbar^2}{2m}\Delta + q(x)\right]\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t) \tag{1}$$

can be considered as the basic object of quantum mechanics. Its solution completely describes a system at all times; that is why it is so important to be able to analyze and solve the Schrödinger equation. Unfortunately, this partial differential equation includes dependence on space and time, makes (1) difficult even for a numerical solution and extremely complicated to examine analytically. Usual methods in such cases are spectral analysis of operators, perturbation theory, and asymptotic methods. But all of them are based on a comparison of properties (spectrum, asymptotics) of two objects (operators, solutions) that are closely related in some sense. One should expect preservation or slight changes in these properties.

Separation of (1) by $\psi(x,t) = e^{-izt/\hbar}u(x)$ into time-dependent only and spatial equations with further reduction of the spatial equation to one dimensional time-independent case ($\hbar = 1,\ m = 1/2$) gives

$$-\frac{d^2}{dx^2}u(x) + q(x)u(x) = zu(x) \tag{2}$$

which is easy to solve only for infinitely smooth potentials $q(x)$ with compact support. In this simple case it is possible to find an infinite asymptotic series for the solution for large energies z:

$$u(x) = exp(i\sqrt{z}x)\sum_{j=0}^{\infty}\frac{Q_j(x)}{\sqrt{z}^j},\ z \to \infty, \tag{3}$$

where $Q_j(x)$ are integrals of the derivatives of the potential q (we leave this as an exercise). Physicists, however, are interested in singular, slowly decaying, or non-smooth potentials (e.g., Coulomb potential $q(x) = 1/x$ is non-integrable at zero and infinity). There is the question of determining the number of terms in the asymptotic representation (3) that can still be calculated if $q \in L_1$ has N integrable derivatives [14]:

$$u(x) = exp(i\sqrt{z}x) \sum_{j=0}^{N+2} \frac{Q_j(x)}{\sqrt{z}^j} + o\left(\frac{1}{\sqrt{|z|}^{N+2}}\right), \quad z \to \infty. \tag{4}$$

There is also the question of finding sufficient condition(s) (written in the simplest or the easiest to apply form) or necessary condition(s) (the most difficult and important problem) to write asymptotics like (4) for slowly decaying potentials (L_2, L_p for $p > 2$).

Next we talk about boundary conditions. We are considering WKB-type asymptotic behavior at infinity (see (8)). Such a choice is reasonable since limit values are the easiest to obtain in experiments and more natural for experimental physics. We prove the existence and uniqueness of the solution to (2) in L_2 for square integrable potentials with integrable first derivative, but this fact is not new. Very similar questions arise in the discrete case. There is a well-known class of Jacobi matrices (discrete string operator) where, again, WKB asymptotics appears (see e.g. [1]).

There are many papers devoted to the trace formulas. We would like to highlight important stages in this field. First, the formulas appeared in the paper by Gel'fand and Levitan in 1953, where the authors obtained some identities for the eigenvalues of a regular Sturm-Liouville operator. These formulas relate the spectrum of an operator to certain characteristics of the operator called trace formulas. A detailed account of trace formulas on finite intervals can be found in Dikii's paper [6]. In 1957 Faddeev considered the case of singular Sturm-Liouville operator which full description were obtained in the paper [3] by Buslaev and Faddeev in 1960 for short-range potentials q (i.e. existence of the first moment of q) with, in addition, q' to be continuous and q' has a finite limit as x tends to infinity. Namely, the first trace formula is:

$$-\sum_{j=1}^{m}\lambda_j + \frac{2}{\pi}\int_0^\infty t\left(\theta(t) - \frac{1}{2t}\int_0^\infty q(x)dx\right)dt = -\frac{1}{4}q(0), \tag{5}$$

where $\{\lambda_j\}$ are eigenvalues of the Schrödinger operator $H = -\Delta + q(x)$ in L_2 with the potential q. The function θ is the limiting phase and is related to the Krein's spectral shift function ξ by $\xi(t) = \pi^{-1}\theta(\sqrt{t})$.

Then, in 1994 Gesztesy and Holden proved the trace formulas for L_1 potentials in [7]. Later, in 1999 Rybkin in [13] found necessary and sufficient conditions in terms of Fourier transformation of the potential for convergence of the first trace formula. He also considered the case of long-range potentials in 1999 in [15] where Rybkin obtained the first trace formula for L_2 potentials. He required four derivatives of the potential to exist. The present paper is an attempt to combine all these results together and improve the methods for the L_2 class of potentials (so-called long-range potentials) with minimal number of integrable derivatives. The integral in (5) can be viewed as a regularization of the first moment of the limiting phase θ. In our case of L_2 potential the integral is divergent. We have found another regularization of the first trace formula (first moment) as well as of trace formulas of higher

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order (higher moments).

Our approach is based on the combination of methods of different authors. First, following Rybkin, we represent the solution to (2) as a series of functions (see (21)), and then using this representation to find asymptotics over the set of $\left\{\frac{1}{\sqrt{z^j}}\right\}_{j=1}^{\infty}$ (see (22)). In order to use Buslaev-Faddeev trace formulas we consider q_n, a smooth cutoff of the potential q. The new potential has compact support that makes it possible to write trace formulas for q_n. The last step is to take the limit when the place of cutoff n tends to infinity (see (35), (36)).

Trace formulas are applied in inverse problem analysis. They do not allow to restore unknown potential by known scattering data. Trace formulas are more like conditions on unknown potential which can test a potential by plugging in the trace relations and either reject or accept it. More information known about the potential a priori more trace formulas can be written. Thus, it is easier to test potentials. Another application of the trace formulas was found by Deift and Killip [5]. They investigated absolutely continuous spectrum of the perturbed operator under perturbation by L_2 potentials (in continuous and discrete cases).

It is amazing that trace formulas are invariants of the well-known Korteweg-de Vriez equation (KdV invariants). KdV equation arose in an approximate theory of hydrodynamic waves and has the following form

$$V_t - 6VV_x + V_{xxx} = 0, \; V(x,0) = V(x) \rightarrow_{|x|\rightarrow\infty} 0. \tag{6}$$

Then the initial value $V(x)$ can be viewed as the potential at the Schrödinger equation

$$-\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = z\psi(x).$$

Trace formulas relate the potential $V(x)$ and some scattering data (the reflection coefficient, eigenvalues) which have simple correspondence with the scattering data for $V(x,t)$. The main conclusion is that the KdV equation is a completely integrable Hamiltonian system and the mapping variable V into the scattering data plays role of a transformation into canonical variables of the type involving angle and action variables ([7], [10]).

Recently, Simon and Zlatos [19] found an unexpected application of trace formulas to some open questions about orthogonal polynomials. A set of orthogonal polynomials corresponds to a Jacobi matrix. Discrete analog of trace formulas (sum rules) provides extra information about the orthogonal polynomials. This application is quite new. Promising also seems to be using trace formulas and the limiting phase as a replacement to the spectral shift function in the case of long-range potentials.

The author would like to thank his advisor A.V.Rybkin for initiating interest in these problems and for multiple discussions that took place during the course of the research. Without his help the work would not be complete.

2 Notation.

Here we describe the notation used in the present paper: $\mathbb{N} = \{1, 2, 3, ...\}$, $\mathbb{R}_+ = (0, \infty)$, $\mathbb{C}_+ = \{z \in \mathbb{C} : Imz > 0\}$, and $\overline{\mathbb{C}_+} = \left(\mathbb{C}_+ \cup \mathbb{R}\right) \backslash \{0\}$. All functions are assumed to be measurable and we denote the following functional classes:

$$L_p(\Delta) := \left\{f : \|f\|_p^p \equiv \int_\Delta |f(x)|^p \, dx < \infty\right\}, \quad 1 \le p < \infty$$

$$L_\infty(\Delta) := \left\{f : \|f\|_\infty \equiv ess \sup_{x \in \Delta} |f(x)| < \infty\right\}.$$

These norms obey the Holder inequality:

$$\|fg\|_r \le \|f\|_p \|g\|_q, \; where f \in L_p, \; g \in L_q, \; and \; 1/r = 1/p + 1/q.$$

And

$$W_1^p(\Delta) := \left\{f : f, f', ..., f^{(p)} \in L_1(\Delta)\right\}, \; 1 \le p < \infty.$$

Furthermore, all Hilbert spaces are assumed to be separable, and for a linear operator A we denote as $\sigma(A)$ the spectrum of A, $\rho(A) = \mathbb{C} \backslash \sigma(A)$ is the resolvent set, $\{\lambda_n(A)\}$ are eigenvalues, $s_k(A) \equiv \lambda_k\left(\sqrt{A^*A}\right)$ are singular numbers of A, and we denote the following ideals of compact operators:

$$\mathcal{S}_p := \left\{A : \|A\|_p^p \equiv \sum_k s_k^p(A) < \infty\right\}, \quad 1 \le p < \infty.$$

There are two important ideals: $\mathcal{S}_1$ or trace class, and $\mathcal{S}_2$ or Hilbert-Schmidt class. The following inequalities show relations between the usual operator norm $\|\cdot\|$ and $\mathcal{S}_1$, $\mathcal{S}_2$ norms:

$$\|A\| \le \|A\|_2 \le \|A\|_1,$$

$$\|AB\|_1 \leq \|A\|\|B\|_1,$$

$$\|AB\|_2 \leq \|A\|\|B\|_2,$$

$$\|AB\|_1 \leq \|A\|_2\|B\|_2$$

for suitable linear operators A, B (see, e.g. [11]).

Another fact provides a practical method for calculating the $\|\cdot\|_2$ norm if the linear operator is an integral operator:

If $(Af)(x) = \int_M K(x,y)f(y)dy$ then A is Hilbert-Schmidt if and only if $K \in L_2(M \times M)$ and

$$\|A\|_2^2 = \int_{M\times M} |K(x,y)|^2 dxdy = \|K\|_2^2.$$

Also, we need to be able to asymptotically compare functions:

$f(x) = O(g(x)), x \to a$ $(-\infty \leq a \leq \infty)$ if

$$\lim_{x\to a}\left|\frac{f(x)}{g(x)}\right| = C, \ \textit{where}\ 0 < C < \infty$$

$f(x) = o(g(x)), x \to a$ $(-\infty \leq a \leq \infty)$ if

$$\lim_{x\to a}\left|\frac{f(x)}{g(x)}\right| = 0$$

For a function f there is an **asymptotic representation (or just asymptotics) over some collection of functions** $\{\varphi_j(x)\}_{j=1}^{N+1}$ in one of the following forms (the first one requires a little more work):

$$f(x) = \sum_{j=1}^{N} c_j\varphi_j(x) + O(\varphi_{N+1}(x)),\ \textit{as}\ x \to a,$$

or

$$f(x) = \sum_{j=1}^{N} c_j\varphi_j(x) + o(\varphi_N(x)),\ \textit{as}\ x \to a,$$

where $\forall\ j\ \varphi_{j+1}(x) = o(\varphi_j(x)),\ as\ x \to a.$

Then the last term $O(\varphi_{N+1}(x))$ $(o(\varphi_N(x)))$ is called the error of the asymptotics. The number of required terms depends on the specific problem.

In fact, if $f_n(x) = \sum_{j=1}^{N} c_j(n)\varphi_j(x) + o(\varphi_N(x))$, $f(x) = \sum_{j=1}^{N} c_j\varphi_j(x) + o(\varphi_N(x))$ are asymptotic representations of the functions f_n, f, as $x \to a$ and $\lim_{n\to\infty} f_n(x) = f(x)$, then it is easy to show that

$$\lim_{n\to\infty} c_j(n) = c_j,\ \forall j.$$

The asymptotics of the limit function is the asymptotics where each coefficient is the limit of old coefficients.

3 The WKB asymptotics.

This section is about the existence, uniqueness and a right representation of the solution to a one dimensional Schrödinger equation with suitable asymptotic behavior at infinity as a boundary condition.

Consider a one-dimensional Schrödinger equation with boundary condition at $x = 0$, $(x \in R_+)$

$$\begin{cases} -u'' + q(x)u = zu, \\ u(0) = 1 \end{cases} \tag{7}$$

According to Weyl theory [12] the equation (7) has unique solution in L_2 for a wide class of potentials. In particular, if q is locally integrable then the solution to (7) $\psi(x, z)$ (Weyl solution) is square integrable for all $z \in \mathbb{C}_+$. We will show that the condition $u(0) = 1$ can be replaced by fixing the asymptotic behavior of the solution for large x. Namely, we will prove the following well-known fact (see, e.g.[4]):

Theorem 1 *If $q \in L_2(R_+)$, $q' \in L_1(R_+)$ then the problem*

$$\begin{cases} -u'' + q(x)u = zu \\ \lim\limits_{x\to\infty} u(x, z) \exp\left(-ix\sqrt{z} - \dfrac{1}{2i\sqrt{z}} \displaystyle\int_0^x q(s)ds\right) = 1 \end{cases} \tag{8}$$

has a unique solution $\forall z \in \overline{\mathbb{C}_+}$.

Remark 1 *Asymptotic behavior of the type* $\exp\left(ix\sqrt{z} + \frac{1}{2i\sqrt{z}} \int_0^x q(s)ds\right)$ *is called WKB type asymptotics. The part "type" in the name can be understood if we assume for a second that q is integrable [16]. Let us consider two solutions:* $\exp(-ix\sqrt{z})$ *and* $\exp\left(ix\sqrt{z} + \frac{1}{2i\sqrt{z}} \int_0^x q(s)ds\right)$. *Since*

$\lim_{x\to\infty}\int_0^x q(s)ds < \infty$ *it follows that these two solution are essentially the same up to a bounded phase factor.*

Proof

The theorem itself is not new. The main result of the proof will be the recursive representation (21) that will be used throughout the paper.
It is usually difficult to find a simple model of the solution to (8) that carries a considerable part of the information about the solution. In our case there is a hint, namely the given asymptotics. For $k=\sqrt{z}\in\mathbb{C}_+$ let

$$\Theta(x,k)=\exp\left(ikx+\frac{1}{2ik}\int_0^x q(s)ds\right). \tag{9}$$

We are going to construct the solution to (8) based on the function Θ. First, we would like to find an equation for Θ similar to (8). Differentiation with respect to x shows that $\Theta(x,k)$ satisfies

$$-\Theta''(x,k)+[q(x)-q_1(x,k)-k^2]\Theta(x,k)=0, \tag{10}$$

where

$$q_1(x,k)=-\frac{q'(x)}{2ik}+\frac{q^2(x)}{4k^2} \tag{11}$$

Rewrite (8) in the form

$$-u''(x,k)+[q(x)-q_1(x,k)-k^2]u(x,k)=-q_1(x,k)u(x,k) \tag{12}$$

and note that (10) is the homogeneous equation for (12). Take $\Theta(x,k)$ and $\Theta(x,k)\int_0^x\Theta^{-2}(s,k)ds$ as a set of fundamental solutions to (10). By variation of parameters, the Weyl solution ψ of (8) can be represented as

$$\psi(x,k)=\Theta(x,k)\left\{1+\int_x^\infty q_1(s,k)\Theta(s,k)\left(\int_x^s\Theta^{-2}(t,k)dt\right)\psi(s,k)ds\right\}. \tag{13}$$

Setting $y = \Theta^{-1}\psi$ and introducing the kernel

$$K(x,s,k) = q_1(s,k)\Theta^2(s,k)\int_x^s \Theta^{-2}(t,k)dt, \tag{14}$$

and then equation (13) reads

$$y(x,k) = 1 + \int_x^\infty K(x,s,k)y(s,k)ds = 1 + (\mathbb{K}y)(x,k). \tag{15}$$

This integral equation is Volterra-type and can be solved by iterations that are convergent, as we show below. The condition $q' \in L_1(\mathbb{R}_+)$ implies (since $q(x) = q(0) + \int_0^x q'(t)dt$) that $q \in L_\infty(\mathbb{R}_+)$. Also, it is clear that $q_1(\cdot,k) \in L_1(\mathbb{R}_+)$, for all $k \in \overline{\mathbb{C}_+}$. We will show $\mathbb{K}$ is a bounded linear operator from L_∞ to L_∞. We need to estimate:

$$\int_x^s \Theta^{-2}(t,k)dt = \int_x^s e^{-2iks}\cdot\exp\left(-\frac{1}{ik}\int_0^t q(z)dz\right)dt. \tag{16}$$

Integration by parts leads to

$$= \left.\frac{\Theta^{-2}(t,k)}{-2ik}\right|_{t=x}^{t=s} + \frac{1}{4k^2}\int_x^s \Theta^{-2}(t,k)q(t)dt \tag{17}$$

and integration by parts a second time leads to

$$= \left.\frac{\Theta^{-2}(t,k)}{-2ik}\right|_{t=x}^{t=s} + \left.\frac{q(t)\Theta^{-2}(t,k)}{-4ik^3}\right|_{t=x}^{t=s} + \frac{1}{4ik^3}\int_x^s \Theta^{-2}(t,k)\left(q'(t) - \frac{q^2(t)}{ik}\right)dt. \tag{18}$$

The last expression estimates by norms of q and q':

$$\left|\int_x^s \Theta^{-2}(t,k)dt\right| \leq \frac{1}{|k|} + \frac{2||q||_\infty + ||q'||_1}{4|k|^3} + \frac{||q||_2}{4|k|^4} \tag{19}$$

Using (14) the following can be derived:

$$||\mathbb{K}|| = \sup_{||f||_\infty=1} ||\mathbb{K}f||_\infty = \sup_{||f||_\infty=1} \sup_{x\in\mathbb{R}} \left| \int_0^\infty K(x,s,k)f(s)ds \right|.$$

Applying Hölder's inequality

$$\leq \sup_{||f||_\infty=1} \sup_{x\in\mathbb{R}} \int_0^\infty |K(x,s,k)|\, ds ||f||_\infty \leq \sup_{x\in\mathbb{R}} \int_0^\infty |K(x,s,k)|\, ds,$$

and using the estimate (19)

$$= \sup_{x\in\mathbb{R}} \int_R |q_1(s,k)| \left| \int_x^s \Theta^{-2}(t,k)dt \right| ds \leq \sum_{j=2}^{6} \frac{C_j}{|k|^j}.$$

So, if $|k| > r := \max_{2\leq j\leq 6}(|5C_j|^{1/j}) > 0$, then $||\mathbb{K}|| < 1$ and the error term in

$$y(x,k) = 1 + \sum_{m=1}^{n} (\mathbb{K}^m 1)(x,k) + (\mathbb{K}^{n+1} y)(x,k) \tag{20}$$

can be evaluated through $||\mathbb{K}||$:

$$||\mathbb{K}^{n+1} y||_\infty \leq ||\mathbb{K}||^{n+1} ||y||_\infty.$$

From (15) and the fact $||\mathbb{K}|| < 1$, we obtain $||y||_\infty \leq \left(1 - ||\mathbb{K}||\right)^{-1}$ and then

$$\leq ||\mathbb{K}||^{n+1} \left(1 - ||\mathbb{K}||\right)^{-1}$$

so $||\mathbb{K}^{n+1} y||_\infty \to 0$ as $n \to \infty$, if $|k| > r$, and hence

$$y(x,k) = 1 + \sum_{n=1}^{\infty} (\mathbb{K}^n 1)(x,k). \tag{21}$$

This representation will be essential to this paper. Since $u = \Theta y$ the theorem is proved.

Remark 2 *Transformation (15) of the Schrödinger equation appears to be new.*

Remark 3 *We represented the solution to (8) in the form* $\psi(x,k) = \Theta(x,k)y(x,k)$ $= \Theta(x,k)\left(1 + \sum_{n=1}^{\infty}(\mathbb{K}^n 1)(x,k)\right)$. *For further calculations we do not need* $\psi(x,k)$ *for all* x*, but only* $\psi(0,k)$ *as a function of* k*. Since* $\psi(0,k) = \Theta(0,k)y(0,k) = y(0,k)$ *and* $y(x,k)$ *has a simpler form this determined our choice of* $y(x,k)$ *as the main object of the paper.*

4 Some key asymptotics.

In this section we find the asymptotic representation of $y(0, k)$ and relate the number of exact terms with the smoothness of the potential q. We use the same idea as in [14], but our kernel $K(x, s, k)$ has a more complex structure. The new kernel requires extensive calculations and careful analysis of each part. The main result of the section is formulated as follows:

Theorem 2 *Let* $q \in L_2(\mathbb{R}_+)$, $q' \in W_1^{N-1}(\mathbb{R}_+)$. *Let* $M(k) = \psi(0, k) = y(0, k)$, *where* $y(x, k)$ *is a defined by (15). Then*

$$M(k) = \sum_{j=0}^{N+2} \frac{m_j}{(ik)^j} + O\left(\frac{1}{|k|^{N+3}}\right), \quad as\ k \to \infty, k \in \overline{\mathbb{C}_+}, \tag{22}$$

where $\{m_j\} \in \mathbb{C}$ *are some constants.*

Remark 4 *We do not compute exact expressions for the coefficients* $\{m_j\}$. *The uniqueness of the function* $M(k)$ *allows us to use the results of Buslaev-Faddeev [3]. The lemma gives only the number of the coefficients that can be calculated with our conditions on the potential. So the fact is, if a square summable potential* q *has* N *summable derivatives then we can calculate* $N+2$ *terms of the asymptotic representation of* $M(k)$ *(we will use values of* $N+2$ *coefficients of the asymptotics of* $M(k)$ *from [3]).*

Below are two technical lemmas which we need for the repeated integration in (21).

Lemma 1 *Let* $q(x)$, $f(x)$ *be functions such that* $q(x) \in L_2(\mathbb{R}_+)$, $q'(x) \in W_1^{m-1}(\mathbb{R}_+)$, *and* $f(x) \in W_1^m(\mathbb{R}_+)$, *for some* $m \geq 1$, *and denote by* D *the* *linear operator:*

$$D = \frac{d}{dx} + \frac{q(x)}{ik}$$

Then $D^j f(\cdot, k) \in L_1(\mathbb{R}_+)$, $\forall\ 1 \le j \le m$.

Proof

We use that $q \in L_\infty$ (see note to (15)) and apply induction.

Lemma 2 *Let* $G(x,s,k) = \Theta^2(s,k)\int_x^s \Theta^{-2}(t,k)dt$. *If* $f \in L_1$ *and* f *is differentiable, then the following formula holds:*

$$\int_x^\infty G(x,s,k)f(s)ds = -\frac{1}{2ik}\int_x^\infty f(s)ds - \frac{1}{2ik}\int_x^\infty G(x,s,k)Df(s,k)ds$$

Proof

Performing integration by parts we find:

$$\int_x^\infty G(x,s,k)f(s)ds = \int_x^\infty e^{2iks}\cdot\exp\left(\frac{1}{ik}\int_0^s q(y)dy\right)\int_x^s \Theta^{-2}(t,k)dt f(s)ds,$$

$$= \frac{G(x,s,k)f(s)}{2ik}\Bigg|_{s=x}^{s\to\infty} - \frac{1}{2ik}\int_x^\infty \left(G(x,s,k)f'(s) + f(s) + G(x,s,k)f(s)\frac{q(s)}{ik}\right)ds.$$

Cancelling the integrated terms, since $G(x,x,k) = 0$, $f \in L_1$ and $G(x,\cdot,k) \in L_\infty$, leads to the desired formula:

$$\int_x^\infty G(x,s,k)f(s)ds = -\frac{1}{2ik}\int_x^\infty f(s)ds - \frac{1}{2ik}\int_x^\infty G(x,s,k)Df(s,k)ds. \tag{23}$$

The conditions $f \in W_1^1(\mathbb{R}_+)$ is necessary for the existence of the integrals in (23).

Remark 5 *Lemma 2 says that it is possible to perform integration by parts if the integrand has the special form $G(x,s,k)f(s)$, with $f \in W_1^1$. Since $q_1 \in W_1^{N-1}$, by Lemma 1, all $Dq_1, D^2q_1, \cdots, D^{N-1}q_1$ are from L_1. Thus they can play the role of f in Lemma 2. We can apply Lemma 2 $N-1$ times and the last integral will still be convergent.*

Let us prove Theorem 2.

Proof

Using the fact that $M(k) = y(0,k)$ and formula (21) we can write down the object whose asymptotic representation as $k \to \infty$ that we would like to find:

$$M(k) = 1 + \sum_{j=1}^{\infty} (\mathbb{K}^j 1)(0,k).$$

By induction, the analysis can be done in 2 steps: full analysis of $\mathbb{K}1$ and analysis of $\mathbb{K}^n 1$.

Consider $G(x,s,k)$. Using (18) one can conclude:

$$\begin{aligned} G(x,s,k) &= \Theta^2(s,k)\left.\frac{\Theta^{-2}(t,k)}{-2ik}\right|_{t=x}^{t=s} + O\left(\frac{1}{k^3}\right) \\ &= \frac{1-\Theta^2(s,k)\Theta^{-2}(x,k)}{-2ik} + O\left(\frac{1}{k^3}\right). \end{aligned} \tag{24}$$

Applying Lemma 2 to the integral $N-1$ times gives:

$$(\mathbb{K}1)(x,k) = \int_x^{\infty} G(x,s,k) q_1(s,k) ds$$

$$= \sum_{j=2}^{N} \frac{d_j(x)}{k^j} + \frac{1}{(-2ik)^{N-1}} \int_x^{\infty} G(x,s,k) D^{N-1} q_1(s,k) ds + O\left(\frac{1}{k^{N+3}}\right).$$

Using (24) one arrives at:

$$(\mathbb{K}1)(x,k) = \sum_{j=2}^{N} \frac{d_j(x)}{k^j} + \frac{\Theta^{-2}(x,k)}{(-2ik)^N} \int_x^\infty D^{N-1} q_1(s,k)ds$$

$$+\frac{\Theta^{-2}(x,k)}{(-2ik)^N} \int_x^\infty \Theta^2(s,k) D^{N-1} q_1(s,k)ds + O\left(\frac{1}{k^{N+3}}\right). \tag{25}$$

The first integral gives two terms with Θ^{-2} (see (26)). Consider the last integral

$$\int_x^\infty \Theta^2(s,k) D^{N-1} q_1(s,k)ds.$$

By Lemma 1, since $D^{N-1}q_1(\cdot,k) \in L_1$, the last integral is convergent. Performing integration by parts, and using (11), this last integral equals

$$\frac{D^{(N-1)}q_1(x)\Theta^2(x,k)}{-2ik} + O\left(\frac{1}{k^3}\right) = \frac{q^{(N)}(x)\Theta^2(x,k)}{(-2ik)^2} + O\left(\frac{1}{k^3}\right).$$

Coming back to (25)

$$(\mathbb{K}1)(x,k) = \sum_{j=2}^{N+2} \frac{d_j(x)}{k^j} + \frac{w_{N+1}(x)\Theta^{-2}(x,k)}{k^{N+1}} + \frac{w_{N+2}(x)\Theta^{-2}(x,k)}{k^{N+2}} + O\left(\frac{1}{k^{N+3}}\right). \tag{26}$$

For $x = 0$ (since $\Theta^{-2}(0,k) = 1$):

$$(\mathbb{K}1)(0,k) = \sum_{j=2}^{N} \frac{d_j}{k^j} + \frac{w_{N+1} + d_{N+1}}{k^{N+1}} + \frac{w_{N+2} + d_{N+2}}{k^{N+2}} + O\left(\frac{1}{k^{N+3}}\right). \tag{27}$$

One can verify that if

$$(\mathbb{K}^n\ 1)(0,k) = \sum_{j=p_0}^{p} \frac{h_j}{k^j} + O\left(\frac{1}{k^{p+1}}\right),\ k \to \infty$$

with some integer $n, p_0,\ p$ then

$$(\mathbb{K}^{n+1}\ 1)(0,k) = \sum_{j=p_0+2}^{p} \frac{w_j}{k^j} + O\left(\frac{1}{k^{p+1}}\right),\ k \to \infty.$$

Now the sum begins at p_0+2. Two additional k come from the noting that in (27) the sum begins at 2 and the iterative relation between $\mathbb{K}^n$ and $\mathbb{K}^{n+1}$ is the following:

$$(\mathbb{K}^{n+1}\ 1)(0,k)=\int_0^\infty K(0,s,k)(\mathbb{K}^n\ 1)(s,k)ds.$$

Thus

$$M(k)=1+(\mathbb{K}1)(0,k)+(\mathbb{K}^2 1)(0,k)+\cdots=1+\sum_{j=2}^{N+2}\frac{m_j}{k^j}+O\left(\frac{1}{|k|^{N+3}}\right),\ k\to\infty.$$

We have obtained the asymptotics for real k. Thus this is true for all $k\in\overline{\mathbb{C}_+}$.

This completes the proof.

Remark 6 *From Theorem 2 follows*

$$\ln M(k)=O\left(\frac{1}{|k|^2}\right),\quad k\to\infty.$$

This explains why in Lemma 4 $Q_1=0$

5 The Spectral shift function.

Here we introduce the spectral shift function. This function is not natural for the Schrödinger operator, but is important for physicists since it can be obtained from experiments. The spectral shift function is related to the scattering matrix and also to the limiting phase that is a part of the trace formulas [17].

Consider (H, H_0) a pair of resolvent comparable operators (i.e., $(H-zI)^{-1} - (H_0 - zI)^{-1} \in \mathcal{S}_1$) for some complex z. Then there exists (see [2]) a unique (up to an additive constant) real-valued function $\xi(k)$ such that $\frac{\xi(k)}{1+k^2}$ is from $L_1(\mathbb{R})$ and such that the Krein trace formula

$$tr\{\varphi(H) - \varphi(H_0)\} = \int_{\mathbf{R}} \varphi'(k)\xi(k)dk$$

holds for all φ from some suitable class. The function $\xi(k)$ is called the spectral shift function of the pair (H, H_0). For almost all k from the absolutely continuous spectrum of H_0, the function $\xi(k)$ is related to the scattering matrix $S(k)$ of (H, H_0) by the Birman-Krein formula [12]:

$$\det S(k) = e^{-2\pi i \xi(k)}.$$

This formula is a generalization of the fact that $\xi(\lambda) = \pi^{-1}\theta(\sqrt{\lambda})$, where θ is the so-called limiting phase.

However, if the difference of resolvents is not from the trace class anymore, then all mentioned above facts are not true. One possible way to deal with such pairs of operators is to follow Koplienko [9] and introduce the regularized spectral shift function η satisfying the regularized trace formula:

$$tr\left\{\varphi(H_0+V)-\varphi(H_0)-\frac{\varphi(H_0+\varepsilon V)}{d\varepsilon}\bigg|_{\varepsilon=0}\right\}=-\int_{\mathbf{R}}\varphi''(k)\eta(k)dk,$$

and η' corresponds (plays the same role as) to ξ.

In [9] Koplienko proved the following fact:

If $\left|\frac{d^j q}{dx^j}\right| \leq (1+|x|)^{-\alpha-j}$ with some $\alpha > 1/2$ and $j = 0, 1, 2$, then there exists the real-valued and bounded from above function η summable over $\mathbb{R}$ with the weight $\frac{1}{(1+t^2)^\gamma}$ for any $\gamma > 1/2$, and such that $\eta'(\lambda) = \pi^{-1}\theta(\sqrt{\lambda})$ for positive λ.

Koplienko considers a smooth cutoff of the potential and uses two facts:

$$\lim_{n\to\infty}\left\|(q-q_n)(H_0-zI)^{-1}\right\|_2=0$$

and

$$\lim_{n\to\infty} M_n(k)=M(k), \forall k\in\overline{\mathbb{C}_+},$$

which we prove below in our conditions on the potential: $q \in L_2(\mathbb{R}_+)$, $q' \in L_1(\mathbb{R}_+)$.

Lemma 3 *Let $q \in L_2$, $q' \in L_1$, define q_n*

$$q_n(x)=\begin{cases} q(x), x\in[0,n] \\ 0, x\in[n+1,\infty)\end{cases}$$

and $\left|\frac{d^j q_n(x)}{dx^j}\right| \leq \frac{C}{n^\alpha}$, $j = 0, 1$ when $x \in [n, n+1]$.
Let $M(k) = u(0,k)$, where $u(x,k)$ is the solution to the problem (8), and $M_n(k) = u_n(0,k)$ with $u_n(x,k)$ to be a solution $-y''+q_n(x)y = k^2y$, satisfying condition like (8). Then:

1. $\lim_{n\to\infty} M_n(k) = M(k), \forall k \in \overline{\mathbb{C}_+},\ |k| > r.$

2. $\lim_{n\to\infty} \left\|(q - q_n)(H_0 - zI)^{-1}\right\|_2 = 0,\ z \in \mathbb{C}\backslash\mathbb{R}.$

3. $\lim_{n\to\infty} \left\|(q - q_n)(H_n - zI)^{-1}\right\|_2 = 0,\ z \in \mathbb{C}\backslash\mathbb{R}.$

where $H_0 = -\frac{d^2}{dx^2}$, $H_n = -\frac{d^2}{dx^2} + q_n(x)$.

Proof

1. Using the definition of $M(k)$

$$|M(k) - M_n(k)| = |u(0,k) - u_n(0,k)| = |y(0,k) - y_n(0,k)|$$

and representation (21)

$$\leq \sum_{j=1}^{N} \left|(\mathbb{K}^j 1)(0,k) - (\mathbb{K}_n^j 1)(0,k)\right| + \left|(\mathbb{K}^{N+1} y)(0,k) - (\mathbb{K}_n^{N+1} y_n)(0,k)\right|$$

breaking up the last term

$$\leq \sum_{j=1}^{N} \left|\left(\mathbb{K}^j - \mathbb{K}_n^j\right) 1(0,k)\right| + \left|\left(\mathbb{K}^{N+1} - \mathbb{K}_n^{N+1}\right) y(0,k)\right| + \left|\mathbb{K}^{N+1}(y - y_n)(0,k)\right|$$

and using trivial transformation of $\mathbb{K}^j - \mathbb{K}_n^j$, we obtain:

$$= \sum_{j=1}^{N} \left|\left(\sum_{p=1}^{j-1} \mathbb{K}_n^p \left(\mathbb{K} - \mathbb{K}_n\right) \mathbb{K}^{j-p-1}\right) 1(0,k)\right|$$

$$+ \left|\left(\sum_{p=1}^{N} \mathbb{K}_n^p \left(\mathbb{K} - \mathbb{K}_n\right) \mathbb{K}^{N-p}\right) y(0,k)\right| + \left|\mathbb{K}^{N+1}(y - y_n)(0,k)\right|.$$

Since the kernels of $\mathbb{K}$ and $\mathbb{K}_n$ are proportional to q_1 then

$$\left|(\mathbb{K} - \mathbb{K}_n) f(x,k)\right| = \left|\int_n^{\infty} \left(K(x,t,k) - K_n(x,t,k)\right) f(t) dt\right| \to_{n\to\infty} 0.$$

Applying argument $\varepsilon/3$ (the last term is small because $||\mathbb{K}|| < 1$):

$$|M(k) - M_n(k)| = \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} = \varepsilon, \ \forall \varepsilon > 0$$

Thus:

$$\lim_{n\to\infty} M_n(k) = M(k), \ \forall k \in \overline{\mathbb{C}_+}, \ |k| > r. \tag{28}$$

The statement need not true for all k. We used $||\mathbb{K}|| < 1$ which is true for $|k| > r$ with some r (see note to (20)).

2. The second part can be proved by using the exact expression for the kernel of the resolvent of H_0 [15]:

$$(H_0 - \lambda I)^{-1} f(x, \lambda) = \frac{1}{i\sqrt{\lambda}} \int_{\mathbf{R}_+} \left(e^{i\sqrt{\lambda}(x+y)} - e^{i\sqrt{\lambda}|x-y|}\right) f(y)dy.$$

Direct integration gives:

$$\left\|(q - q_n)(H_0 - \lambda I)^{-1}\right\|_2$$

$$= \frac{1}{|\lambda|} \int_0^\infty |q(x) - q_n(x)|^2 \int_0^\infty \left|e^{i\sqrt{\lambda}(x+y)} - e^{i\sqrt{\lambda}|x-y|}\right|^2 dydx.$$

Consider the inner integral

$$\int_0^\infty \left|e^{i\sqrt{\lambda}(x+y)} - e^{i\sqrt{\lambda}|x-y|}\right|^2 dy.$$

Let $\alpha = Im\sqrt{\lambda} \geq 0$ then

$$\leq \int_0^\infty \left(e^{-2\alpha(x+y)} + e^{-2\alpha|x-y|} + 4e^{-\alpha(x+y)}e^{-\alpha|x-y|}\right) dy \tag{29}$$

$$= \int_0^\infty \left(e^{-2\alpha(x+y)} + e^{-2\alpha|x-y|} + 4e^{-\alpha(x+y)}e^{-\alpha|x-y|}\right) dy$$

breaking up into two integrals

$$= \int_0^x \left(e^{-2\alpha(x+y)} + e^{-2\alpha(x-y)} + 4e^{-2\alpha x} \right) dy$$

$$+ \int_x^\infty \left(e^{-2\alpha(x+y)} + e^{-2\alpha(y-x)} + 4e^{-2\alpha y} \right) dy.$$

Evaluating both integrals and estimating the result since αx is positive and $max(4xe^{-2\alpha x}) = \frac{2}{e\alpha} < \frac{2}{\alpha}$

$$= \frac{1}{\alpha} \left(1 + 2e^{-2\alpha x} \right) + 4xe^{-2\alpha x} < \frac{5}{\alpha}.$$

Then the right-hand side of (29) can be estimated as

$$\frac{1}{|\lambda|} \int_0^\infty |q(x) - q_n(x)|^2 \frac{5}{\alpha} dx = \frac{5}{|\lambda Im\sqrt{\lambda}|} \|q - q_n\|_2^2 \to_{n\to\infty} 0.$$

3. Follows from the previous part and simple algebra:

$$(H_n - zI)^{-1} - (H_0 - zI)^{-1}$$

$$= (H_n - zI)^{-1}(H_0 - zI)(H_0 - zI)^{-1} - (H_n - zI)^{-1}(H_n - zI)(H_0 - zI)^{-1}$$

$$= (H_n - zI)^{-1}(H_0 - H_n)(H_0 - zI)^{-1} = -(H_n - zI)^{-1} q_n (H_0 - zI)^{-1}$$

or

$$(H_0 - zI)^{-1} = (H_n - zI)^{-1}(I + q_n(H_0 - zI)^{-1})$$

and then

$$\left\|(q - q_n)(H_n - zI)^{-1}\right\|_2 = \left\|(q - q_n)(H_0 - zI)^{-1}(I + q_n(H_0 - zI)^{-1})^{-1}\right\|_2$$

$$\leq \left\|(I + q_n(H_0 - zI)^{-1})^{-1}\right\| \left\|(q - q_n)(H_0 - zI)^{-1}\right\|_2$$

From $z \in \mathbb{C}\backslash\mathbb{R}$ follows that $z \in \rho(H_n)$. Hence the first norm is finite and, by part 2 of this lemma, the second norm goes to zero.

The lemma is proven.

Corollary 1 *Under assumption of the previous lemma*

$$\lim_{n\to\infty} \left\|(H - zI)^{-1} - (H_n - zI)^{-1}\right\|_2 = 0, \ \forall z \in \mathbb{C}\backslash\mathbb{R}$$

Proof

$$\begin{aligned}\left\|(H - zI)^{-1} - (H_n - zI)^{-1}\right\|_2 &= \left\|(H - zI)^{-1}(H_n - H)(H_n - zI)^{-1}\right\|_2 \\ &\leq \left\|(H - zI)^{-1}\right\| \left\|(q - q_n)(H_n - zI)^{-1}\right\|_2 .\end{aligned}$$

By Lemma 3 the second norm goes to zero, and since $z \in \rho(H)$, the other norm is finite.

This corollary will be used to prove convergence of the trace formulas.

6 Trace formulas.

This section contains the main results of the paper, particularly, (33) and (34). They are the so-called Buslaev-Faddeev trace formulas. In the original paper by Buslaev-Faddeev [3] were used the function η, the so-called limiting phase which is related to our function θ by the following:

$$\theta_{our}(k) = \eta_{Buslaev-Faddeev}(k) - \frac{1}{2k}\int_0^\infty q(t)dt \tag{30}$$

with such a simple relation we can use all results from [3] with slight modifications. Such regularization of the function η is needed in order for the first trace formula to exist. The main method we are applying is to consider a smooth cutoff of the potential at $x = n$, which has compact support and for which all formulas are valid. The next step is taking the limit as n goes to infinity. We will show that the trace formulas still hold.

Lemma 4 *Let $M(k) = A(k)e^{i\theta(k)}$ where $A(k) = |M(k)|$. Suppose that for $x > 0$ $q \in L_2$ and $q' \in W_1^{N-1}$. Then the following formulas hold:*

$$\theta(k) = \sum_{\mu=1}^{[(N+1)/2]} \frac{(-1)^{\mu+1}}{(2k)^{2\mu+1}} Q_{2\mu+1} + O\left(\frac{1}{|k|^{N+3}}\right), k \to \infty, k \in \mathbb{R}, \tag{31}$$

$$\ln A(k) = \sum_{\mu=1}^{[(N+2)/2]} \frac{(-1)^{\mu+1}}{(2k)^{2\mu}} Q_{2\mu} + O\left(\frac{1}{|k|^{N+3}}\right), k \to \infty, k \in \mathbb{R}, \tag{32}$$

where

$$V_0(z) = 0,\ \ V_l(z) = q^{(l-1)}(0) + \sum_{m=1}^{l-1} C_{l-1}^m \int_0^z V_m(t) q^{(l-m-1)}(t)dt$$

$$Q_p = \lim_{z\to\infty}\left(V_{p-1}(z) + \sum_{j=1}^{p-2}\frac{j}{p}V_{p-j-1}(z)Q_j\right)$$

and particularly:

$$Q_1 = 0,\ Q_2 = q(0),\ Q_3 = q'(0) + \int_0^\infty q^2(t)dt,\ Q_4 = q''(0) - 2q^2(0).$$

Proof

Follows from [3] and the uniqueness of $M(k)$.

Theorem 3 *(Trace formulas)*

Let $M(k) = A(k)e^{i\theta(k)}$ where $A(k) = |M(k)|$. Suppose that for $x > 0$ $q \in L_2$ and $q' \in W_1^{N-1}$ then the following formulas are valid:

$$(-1)^\mu \sum_{l=1}^{\infty}\lambda_l^\mu + \frac{2\mu}{\pi}\int_0^\infty t^{2\mu-1}\left[\theta(t) - \sum_{l=1}^{\mu-1}\frac{(-1)^{l+1}}{(2t)^{2l+1}}Q_{2l+1}\right]dt$$
$$= (-1)^\mu\frac{\mu}{2^{2\mu}}Q_{2\mu},\quad 2 \le \mu \le \frac{N+1}{2}; \tag{33}$$

$$(-1)^\mu \sum_{l=1}^{\infty}\lambda_l^{\mu+1/2} - \frac{2\mu+1}{\pi}\int_0^\infty t^{2\mu}\left[\ln A(t) - \sum_{l=1}^{\mu}\frac{(-1)^{l+1}}{(2t)^{2l}}Q_{2l}\right]dt$$
$$= (-1)^\mu\frac{2\mu+1}{2^{2\mu+1}}Q_{2\mu+1},\quad 2 \le \mu \le \frac{N}{2}; \tag{34}$$

Proof

Similar to the proof of Lemma 3, we introduce $q_n(x)$ and corresponding $\theta_n(k)$ and $A_n(k)$. These functions are zero from $x = n+1$, and hence for them the formulas (33) and (34) are valid due to [3].

We can take the limit in the formulas as n approaches infinity:

$$\lim_{n\to\infty}(-1)^\mu \sum_{l=1}^{\infty}\lambda_l^\mu(n) + \lim_{n\to\infty}\frac{2\mu}{\pi}\int_0^\infty t^{2\mu-1}\left[\theta_n(t) - \sum_{l=1}^{\mu-1}\frac{(-1)^{l+1}}{(2t)^{2l+1}}Q_{2l+1}(n)\right]dt$$

$$= \lim_{n\to\infty} (-1)^\mu \frac{\mu}{2^{2\mu}} Q_{2\mu}(n), \quad 2 \le \mu \le \frac{N+1}{2}; \tag{35}$$

$$\lim_{n\to\infty} (-1)^\mu \sum_{l=1}^{\infty} \lambda_l^{\mu+1/2}(n) - \lim_{n\to\infty} \frac{2\mu+1}{\pi} \int_0^\infty t^{2\mu} \left[\ln A_n(t) - \sum_{l=1}^{\mu} \frac{(-1)^{l+1}}{(2t)^{2l}} Q_{2l}(n) \right] dt$$

$$= \lim_{n\to\infty} (-1)^\mu \frac{2\mu+1}{2^{2\mu+1}} Q_{2\mu+1}(n), \quad 2 \le \mu \le \frac{N}{2}. \tag{36}$$

1. It follows from Lemma 3 that $\lim_{n\to\infty} Q_j(n) = Q_j$, for all j.

2. It can be derived from [9] that $\eta_n \to \eta$ in L_1 with weight $\frac{1}{(1+x^2)^\gamma}$, $\gamma > 1/2$. Hence in $L_1(0,a)$ sense with some positive a. Since $\theta(t) = \eta'(t)$ then $t\theta(t) \in L_1(0,a)$ and $t\theta_n(t) \to t\theta(t)$ in $L_1(0,a)$ sense. Thus, to change the integral and the limit in (35) and (36) it is enough to show uniform boundness over (a, ∞) with an integrable bound.

By (31) for all $2 \le \mu \le (N+1)/2$

$$t^{2\mu-1} \left[\theta_n(t) - \sum_{l=1}^{\mu-1} \frac{(-1)^{l+1}}{(2t)^{2l+1}} Q_{2l+1}(n) \right] = \frac{(-1)^{\mu+1}}{2^{2\mu+1} t^2} Q_{2\mu+1}(n) + O\left(\frac{1}{|t|^4}\right)$$

$$\le \frac{C}{t^2} + O\left(\frac{1}{|t|^4}\right), t \to \infty,$$

which is from $L_1(a, \infty)$, with some positive a.

By (32) for all $2 \le \mu \le N/2$

$$t^{2\mu} \left[\ln A(t) - \sum_{l=1}^{\mu} \frac{(-1)^{l+1}}{(2t)^{2l}} Q_{2l}(n) \right] = \frac{(-1)^\mu}{2^{2\mu+2} t^2} Q_{2\mu+2}(n) + O\left(\frac{1}{|t|^4}\right)$$

$$\le \frac{C}{t^2} + O\left(\frac{1}{|t|^4}\right), t \to \infty,$$

which is from $L_1(a, \infty)$, with some positive a.

By Lebesgue's Dominated Convergence Theorem, the limit and integral in (35) and (36) are interchangeable.

3. Consider C as a contour around some interval $[a, b]$, where $a < b < 0$ and a, b are not points of the spectrum of H, then

$$\sum_{\lambda_j(n), \lambda_j \in [a,b]} (\lambda_j(n) - \lambda_j)^2 = \left\| H_n^- - H^- \right\|_2^2,$$

where H^-, H_n^- are spectral projections of H and H_n corresponding to the interval $[a, b]$, where the spectra of H, H_n are discrete, then

$$= \left\| \frac{1}{2i\pi} \int_C \lambda \left(R_\lambda(H) - R_\lambda(H_n) \right) d\lambda \right\|_2^2,$$

where we are estimating the integrand and applying Corollary 1. Finally, we obtain

$$\sum_{\lambda_j(n), \lambda_j \in [a,b]} (\lambda_j(n) - \lambda_j)^2 \leq C \left\| R_\lambda(H) - R_\lambda(H_n) \right\|_2^2 \to 0.$$

This concludes

$$\lim_{n \to \infty} \sum_{\lambda_j(n), \lambda_j \in [a,b]} (\lambda_j(n) - \lambda_j)^2 = 0, \tag{37}$$

where, since $[a, b]$ does not contain 0, the sum is finite.

From Lieb-Thirring bounds [8] $\sum_j (-\lambda_j)^{3/2} \leq \frac{3}{16} \|q\|_2^2 < \infty$, hence

$$\sum_j \lambda_j^2 < \infty. \tag{38}$$

Let $q_-(x)$ be the negative part of the potential, thus $q_-(x) \leq q_n(x)$ for all $x \in \mathbb{R}_+$, then $\lambda_j^- \leq \lambda_j(n)$, where λ_j^- are eigenvalues of the Schrödinger operator with the potential $q_-(x)$. Since all eigenvalues are negative $\left(\lambda_j^-\right)^2 \geq (\lambda_j(n))^2$

then $\sum_j \left(\lambda_j^-\right)^2$ is convergent by the same reasoning as for $\sum_j \lambda_j^2$ mentioned above. This concludes that $\sum_j \lambda_j^2(n)$ is convergent and there is a uniform bound:

$$\sum_j \lambda_j^2(n) \leq \sum_j \left(\lambda_j^-\right)^2 < \infty. \tag{39}$$

Consider

$$\begin{aligned}
&\left|\sum_{\lambda_j(n),\lambda_j\in[a,b]} (\lambda_j^2(n) - \lambda_j^2)\right| \\
&\leq \sum_{\lambda_j(n),\lambda_j\in[a,b]} (\lambda_j(n)-\lambda_j)^2 + 2 \sum_{\lambda_j(n),\lambda_j\in[a,b]} |\lambda_j(\lambda_j(n)-\lambda_j)| \\
&\leq \sum_{\lambda_j(n),\lambda_j\in[a,b]} (\lambda_j(n)-\lambda_j)^2 + 2\sqrt{\sum_{\lambda_j\in[a,b]} (\lambda_j)^2}\sqrt{\sum_{\lambda_j(n),\lambda_j\in[a,b]} (\lambda_j(n)-\lambda_j)^2}.
\end{aligned}$$

Taking the limit as n goes to infinity (all three sums are finite) and using (37) we conclude:

$$\lim_{n\to\infty} \sum_{\lambda_j(n)\in[a,b]} \lambda_j^2(n) = \sum_{\lambda_j\in[a,b]} \lambda_j^2. \tag{40}$$

Then the sums over all eigenvalues represents as the sum of eigenvalues from $[a,b]$ and the rest:

$$\begin{aligned}
\sum_j(\lambda_j^2(n)-\lambda_j^2) &= \sum_{\lambda_j(n),\lambda_j\in[a,b]} (\lambda_j^2(n)-\lambda_j^2) + \sum_{\lambda_j(n),\lambda_j\notin[a,b]} (\lambda_j^2(n)-\lambda_j^2) \\
&= \sum_{\lambda_j(n),\lambda_j\in[a,b]} (\lambda_j^2(n)-\lambda_j^2) + \sum_{\lambda_j(n)\notin[a,b]} \lambda_j^2(n) - \sum_{\lambda_j\notin[a,b]} \lambda_j^2.
\end{aligned} \tag{41}$$

The first term is small because of (40), and the second sum could be split up into two sums since each of them by (38), (39) is convergent and can be made small by the choice of the interval $[a,b]$. Notice that by (39) we can choose $\sum_{\lambda_j(n)\notin[a,b]} \lambda_j^2(n)$ to be small for all n with the same constant. Applying $\varepsilon/3$ argument, then (41) estimates by

$$< \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} = \varepsilon, \ \forall \varepsilon > 0.$$

Thus

$$\lim_{n\to\infty}\sum_j \lambda_j^2(n) = \sum_j \lambda_j^2,$$

and the theorem is proved.

Remark 7 *Particularly:*

$$Q_1 = 0,\ Q_2 = q(0),\ Q_3 = q'(0) + \int_0^\infty q^2(t)dt,\ Q_4 = q''(0) - 2q^2(0).$$

for $\mu = 1$

$$\sum_{l=1}^{\infty}\lambda_l^2 + \frac{4}{\pi}\int_0^\infty t^3\left[\theta(t) - \frac{Q_3}{(2t)^3}\right]dt = \frac{1}{8}Q_4$$

This formula is convergent if the potential q *has the integrable first three derivatives (i.e.* $q \in L_2,\ q', q'', q''' \in L_1$*).*

$$\sum_{l=1}^{\infty}\lambda_l^{5/2} - \frac{5}{\pi}\int_0^\infty t^4\left[\ln A(t) - \frac{Q_2}{(2t)^2} + \frac{Q_4}{(2t)^4}\right]dt = \frac{5}{32}Q_5$$

This formula requires additionally $q^{(4)} \in L_1$.

Formally we could write one additional formula for both functions θ *and* $\ln A$ *(as well as to write trace formulas for* $\mu = 1$*), but we would not be able to prove the convergence of the integrals (or series of negative eigenvalues).*

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